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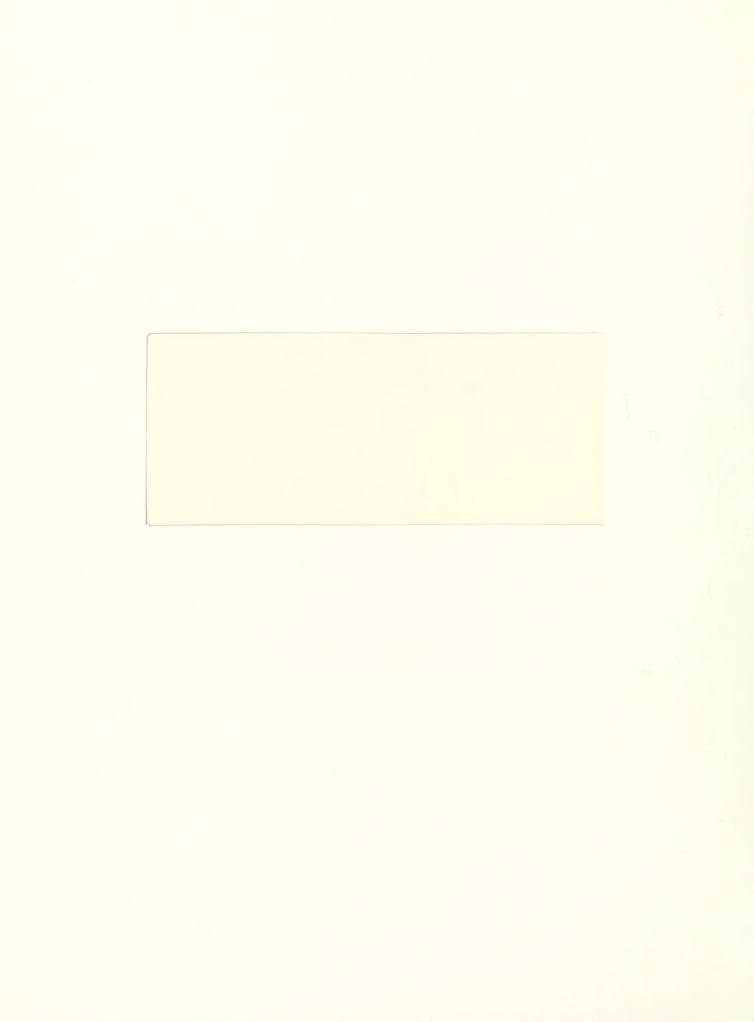
A Sequential Approach of Estimating Two-factor Interactions

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Bin Zhou and Yue Fang

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A Sequential Approach Of Estimating Two-factor Interactions

Bin Zhou Sloan School of Mangement, MIT, Cambridge, MA 02139

Yue Fang Operations Research Center, MIT, Cambridge, MA, 02139

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Abstract

Most literature in fractional factorial design is devoted to studying the main effects of control factors. Recent studies in strategic planning and concurrent engineering deal with completely different problems. In designing a parallel process, knowing interactions among factors, rather than main effects, is even more important. For a large number of control factors, resolution V fractional factorial design is often large and difficult to find. This paper suggests a sequential procedure to estimate all two-factor interactions. The procedure, in the worst scenario, requires n^2+4n-8 experimental runs. The number of experimental runs can be reduced substantially if some prior knowledge of the system is available. The proposed procedure utilizes a series of modified resolution IV designs and provides a systematic approach to construct high resolution experiment designs for any large systems.

1 Introduction

In designing and strategic planning of a complex system, one often needs to know interactions of many potential factors. For example, in concurrent product and process design, the objectives are to consider simultaneously all elements of the product development cycle. Understanding of the interactive relationships among design parameters will help in optimizing the product or process design. In marketing, knowing the interactive relationships among the different features of a line of products will help to reduce the competition among the products themselves. In designing, knowing interactions among different parameters will help to creat more parellel designs. In manufacturing, when a system needs constant calibration, knowing interactions among different control factors will help to optimize the calibration procedure. The common feature of these problems is that understanding of all significant interactions is essential for developing an optimal system.

Most existing research on two-level experiment design concentrate on estimating main effects. When all two and higher order interactions are negligible, the fractional factorial and two-level orthogonal P-B designs are two popular resolution III designs. When two-factor interactions are present, resolution IV designs are needed to estimate main effects. Webb(1968) and Margolin (1969) proved that the minimum number of runs required for n factor resolution IV designs is 2n. To estimate some two-factor interactions in addition to main effects, resolution V designs may be needed. Resolution V designs often require a large number of experimental runs. Box and Hunter (1961(b))gave the smallest resolution V designs for less than seven (7) control factor. Addelman (1965) constructed a resolution V design for 17 factors with 2^{17-9} runs. Some of the known results related to orthogonal resolution III, IV and V designs are shown in Table 1.

Many statistical softwares provide resolution III and IV designs to a considerably large number of experimental parameters. However, the complex structure of resolution V designs makes generating resolution V designs for a large number of control factors extremely difficult. For large system, there is no general systematic method to construct two-level orthogonal resolution V designs except for full fractional designs. This paper proposes a sequential design procedure using the available resolution IV design to estimate all two-factor interactions involved one factor at a time. For n factors, this procedure needs at most $n^2 + 4n - 8$ experimental runs to have all interactions estimated. Main effects can also be solved from confounding patterns. Because it is a sequential method, any knowledge about interaction can be used to reduce experimental runs.

This paper is organized as follows. Section 2 describes how to use resolution V design to estimate all interactions involving one factor. Section

Table 1: Minimum Number of Experimental Runs Required in Orthogonal Designs

Number of Factors	Resolution III	Resolution IV	Resolution V (1)
4	8	8	16
5	8	16	16
6	8	16	32
7	8	16	64
8	16	16	64
9	16	$24^{(2)}$	128
10	16	$24^{(2)}$	128
11	16	$24^{(2)}$	128

(1) For fractional factorial designs only

(2) For fractional factorial designs the number of minimum runs are 32

3 presents a sequential approach of estimating all two-factor interactions. Section 4 presents some simulation results of the proposed procedures.

2 Estimating Two-factor Interactions by Resolution IV Design

Consider the following model

$$Y = \mu + \beta X + X^T A X + \epsilon$$

where $X = (X_1, X_2, ..., X_n)^T$ with values 1 or -1, and ε is a term including the cumulative effect of other variables not included in the model and some random noises. Assume that ε is normal distributed with mean zero and constant variance σ^2 and the different ε 's in each experiment are uncorrelated. μ , vector β and matrix A are the coefficients associated with grand mean, main and interaction effects, respectively. The diagonal entries of matrix A are zeros.

We introduce Interaction Structure Matrix (ISM) which is characterized by vector β and matrix A in the above model. The ISM is an $n \times n$ symmetric matrix that off-diagonal entries (i,j) are a_{ij} 's and diagonal entries (i,i) are β_i 's. Estimating all entries in ISM needs at least n(n+1)/2 experiment runs. Our approach is to estimate one row at a time by modifying

an orthogonal resolution IV design. Assume that we are interested in investigating the main effect of X_1 and all two-factor interactions involving X_1 , that is $X_1X_2, X_1X_3, \ldots, X_1X_n$. We first redefine these effect as $Z_1 = X_1$ and $Z_i = X_1X_i$, i = 2, ..., n. Applying resolution IV design on Z_i 's, we can easily identify all effect of Z_i 's free from all interaction effects of Z_i 's. We noticed that any two-factor interaction of X_i 's are either main effect of Z_i or one of two-factor interaction of Z_i 's. Therefore, we can estimate all effects of $X_1, X_1X_2, X_1X_3, \ldots, X_1X_n$ free from other main and interaction effects of X_i 's.

For an $n \pmod 4$ factor, minimum resolution IV design is foldover Plackett and Burman design. It requires 2n experiment runs. Therefore, we have the following theorem:

Theorem 1 There exists a balanced orthogonal design which estimates independently the main effect X_i and all interactions involving X_i with 2n experimental runs ($n = mod \ 4$ and n < 268). Futhermore, this is a minimum balanced orthogonal design.

The proof is given in the Appendix.

When n is not a module of 4, we use a larger available resolution IV design. For example, if n = 11, we use a resolution IV design with 24 runs without the last column in design matrix.

An example (see Figure 1 and Figure 2) demonstrates how to construct a design to estimate $X_1, X_1X_2, \ldots, X_1X_n$ for n = 12. The first step is to use a cyclic shifting method to obtain Hadamard matrix of order 12 and foldover the matrix to get 24×12 design matrix. Associate each column of the obtained matrix to the main effect X_1 and all interested 11 interactions respectively, as in Figure 1.

To obtain the design matrix for all X_i 's, we multply each column with the first one. The resulting design matrix is shown in Figure 2.

$\int X_1$	X_1X_2	X_1X_3	X_1X_4	X_1X_5	X_1X_6	X_1X_7	X_1X_8	X_1X_9	$X_1 X_{10}$	X_1X_{11}	X_1X_{12}
+	+	+	+	+	+	+	+	+	+	+	+
+	+	-	+	+	+	_	_	_	+	-	-
+	_	+	_	+	+	+	-		_	+	-
+	_	_	+	_	+	+	+	_	_	_	+
+	+	_	_	+	_	+	+	+	_	_	_
+	-	+	_	_	+	_	+	+	+	_	_
+	_		+	_	_	+	_	+	+	+	-
+	_	_	_	+	_	_	+	_	+	+	+
+	+	_	_	_	+	_	-	+	_	+	+
+	+	+	_	_	_	+	_	_	+	-	+
+	+	+	+	-	_	_	+	_	_	+	
+	_	+	+	+	_	_	_	+	_	_	+
-	_	_	-	_	_	_	_	-	_	_	-
-	+	+	_	_	_	+	+	+	_	+	+
_	_	_	+	_	_	_	+	+	+	-	+
-	+	+	_	+	-	_	_	+	+	+	
_	_	+	+	_	+	-	_	_	+	+	+
_	+	_	+	+	_	+	_	_	_	+	+
_	+	+		+	+	_	+	_	_	_	+
_	+	+	+	_	+	+	-	+	_	_	-
_		+	+	+	_	+	+	_	+	_	_
_	_	_	+	+	+	_	+	+	_	+	_
_	_	_	_	+	+	+		+	+	_	+
-	+	_	_	_	+	+	+	_	+	+	-
]

Figure 1: Primary Design Matrix

Figure 2: Design Matrix

3 A Sequential Approach to Estimate All Twofactor Interactions

To estimate all interactions, we use a sequential procedure and estimate interactions involving one factor at a time. At ith step, we focus on estimating all interactions involving ith control factor. Since all interaction effects of X_i with $X_j, j < i$ has been estimated in previous steps, we set them as constants in design matrix and use the procedure described in Section 2 for $X_i, X_i X_{i+1}, \ldots, X_i X_n$. As result, all $X_i X_j, j < i$ are confounded with main effect X_i and $X_i X_j, j > i$ can be estimated free from the other interactions. The main effect can be solved from the confounding structure if necessary. In case of n = 12, the first step needs 24 runs, and so do the second, third and fourth. In the fifth, sixth, seventh and eighth steps, 16 runs for each are required. The remaining three steps need 8, 8 and 4 runs. There are total 180 runs. In general, at most $n^2 + 4n - 8$ runs are needed to carry out the procedure for the n-factor experiment.

Theorem 2 By conducting a series of resolution IV design given in Theorem 1, estimates can be made of all main effects and two-factor interactions with less than $n^2 + 4n - 8$ experimental runs.

The proof is in Appendix.

In the above procedure, main effects are estimated from solving confounding structures. One may argue that the estimation of main effects is affected by the confounding. As we mentioned at the beginning of the paper, we focus more on interactions than main effects. Besides only few interactions are significant in practice (Box & Meyer 1985), therefore we shall be able to have reasonable estimates of all main effects.

In many cases, engineers may have partial knowledge of interaction. They may know that some interactions are zero prior to the experiment. Such prior information can be used in our sequential procedure to further reduce experiment runs. In any step, when an interaction is known to be insignificant, we can set this interaction confounded to main effect. Therefore we may save some runs. In this case, we may also manipulate the order of steps to avoid wasting runs due to the constraint of module 4. The following algorithm explains our strategies:

	\mathcal{X}_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}	X_{11}	X_{12}
X_1	*	X	X	X	X	X	X	X	\mathcal{X}	X	X	0
X_2	\mathcal{X}	*	\mathcal{X}	1.	X	X	X	X	0	0	0	0
X_3	X	X	*	X	-X		X	X	.X	X	0	0
X_4	X	X	\mathcal{X}	*	0	0		0	0	0	0	0
X_5	X	X	\mathcal{X}	0	*	X	\mathcal{X}	-X	X	X	X	-X
X_6	X	X	\mathcal{X}	()	\mathcal{X}	*	\mathcal{X}	0	X	0	0	0
X_7	X	X	X	\mathcal{X}	-X	X	*	0	0	0	0	0
X_8	X	X	X	0	X	0	0	*	0	0	0	0
X_9	X	0	X	0	\mathcal{X}	X	0	0	*	0	0	0
X_{10}	X	()	X	()	\mathcal{X}	0	()	0	0	*	0	0
X_{11}	\mathcal{X}	()	()	()	X	()	0	()	0	()	*	0
X_{12}	0	()	()	()	-X	0	()	()	()	0	0	*

Figure 3: ISM Matrix

Algorithm

- For each unestimated row of ISM, count the number of unestimated main effects and interactions excluding known insignificant interactions and denote it as k_i . Choose the first row of those with the smallest value of $k_i \pmod{4}$.
- Use resolution IV design described in the last section to estimate all interactions for the chosen row.
- Repeat the last two steps until all entries in ISM have been estimated.

We use an example to explain our algorithm. Suppose that we have the ISM given in Figure 3.

All unknown interactions are marked X and known insignificant interactions are marked 0. Fifty percent of the interactions of this ISM are known to be insignificant. The 12 parameters are labelled X_1, \ldots, X_{12} . The first step is to count k_i , which are 11, 8..... We choose and estimate the second row first. Set factors X_9, X_{10}, X_{11} and X_{12} all equal to constant (1 or -1), then we estamate seven interactions involving X_2 with 16 runs. In the second round, we have $k_1 = 10, k_3 = 9, k_4 = 4, \ldots$ Therefore the fourth row is chosen. Set factors $X_2, X_5, X_6, X_8, X_9, X_{10}, X_{11}$ and X_{12} all equal to constant

Table 2: Trace in Solving ISM(1)

Step	Row No.	Runs Needed
1	2	16
2	4	8
3	3	16
4	1	16
5	6	8
6	5	16
Total		80

(1 or -1), then we can estimate three interactions involving X_4 with 8 runs. The process of our procedure is summarized in Table 2.

After six rounds of experiments, only six main effects remain unestimated. Using prior information, we reduce the number of runs to 80, which is less than half of runs needed for a full ISM. There are many ways to set the experimental levels for the factors which are to be kept constant in some rounds. One way to do it is to randomly choose a high or low level for each such factor for the particular round; or, to set the factor level according to the results provided by the previous round. We may also consider other strategies in order to minimize the total number of experimental runs or to minimize the total number of level changes for some or all factors.

In all cases there are possible repeated runs in the experiment. For example, if we set all constant factors to be 1, there are 6 repeated runs performed during the six round experiment. After deleting all repeated experimental runs the total number of runs is only 74 in the above 12 factor experiment.

To find out how many runs are needed in the proposed procedures, we did the following simulation when ISM is known to be sparse. For n factors and different sparses, we generate 1,000 fSM's by randomly placing $p \times 100\%$ of off-diagnal entries non-zero. For n=6,...,20 and p=25%,50%,75%, we calculated the average required experiment runs (without considering repeated runs). The results are listed in Table 3.

In general if m interaction effects needed to be estimated, our procedure would require a little bit more than 2m runs.

Table 3: The numbers of experimental runs needed in the sequential approaches

Factors	P = 25%	P=50%	P=75%
6	$11.3 \ (1.5^{(1)})$	21.8 (2.2)	32.2 (1.1)
7	17.3 (1.9)	29.8(2.4)	46.0 (2.5)
8	23.6(2.4)	41.6(2.7)	65.3 (9.6)
9	29.4 (2.7)	51.3 (3.5)	78.6 (7.5)
10	34.4(2.8)	63.2 (4.1)	91.4 (4.3)
11	40.6 (3.5)	76.2 (5.6)	110.3 (7.4)
12	48.6 (2.7)	89.2 (5.1)	127.2 (8.9)
13	56.4 (3.3)	103.9 (6.3)	148.6 (5.1)
14	63.4 (3.4)	117.8 (5.6)	170.1 (7.8)
15	75.2 (3.4)	134.1 (5.1)	193.2 (9.4)
16	85.4 (3.6)	152.7 (6.1)	218.8 (8.1)
17	95.8 (4.5)	170.2 (5.6)	245.8 (5.4)
18	105.3 (4.4)	188.2 (4.8)	273.1 (7.0)
19	116.7 (4.6)	207.6 (5.2)	300.3 (6.0)
20	128.4 (5.4)	229.9 (5.4)	328.9 (7.5)

⁽¹⁾ Standard Devriations are given in parenthese;

Table 4: Trace of the Six-round Design Strategy for Model(2)

Step	Row No.	Estimated Interactions
1	2	$X_1X_2, X_2X_3, X_2X_4, X_2X_5, X_2X_6, X_2X_7, X_2X_8$
2	4	X_1X_4, X_3X_4, X_4X_7
3	3	$X_1X_3, X_3X_5, X_3X_6, X_3X_7, X_3X_8, X_3X_9, X_3X_{10}$
4	1	$X_1X_5, X_1X_6, X_1X_7, X_1X_8, X_1X_9, X_1X_{10}, X_1X_{11}$
5	6	X_5X_6, X_6X_7, X_6X_9
6	5	$X_5X_7, X_5X_8, X_5X_9, X_5X_{10}, X_5X_{11}, X_5X_{12}$

4 Simulation Results

To further test our procedure, we simulated a system with the following structure

$$y = 2 + 4x_1 + 4x_2 + 3x_3 + 3x_4 + 3x_5 + 2x_6 + 2x_7 + x_8 + x_9 + x_{10}$$

$$+ .5x_{11} + .1x_{12} + x_1x_2 + .5x_1x_3 + .4x_1x_{11} + .3x_2x_4 + .2x_2x_6$$
(1)
$$+ .1x_3x_4 + .1x_6x_7 + \epsilon$$

where ϵ is a random normal variable with mean zero and standard deviation $\sigma=0.1$ We also assumed that prior knowlage of ISM has form in Figure 3. We conducted 80 runs with two replications for each run. During each of six rounds we randomly chose the levels for the factors which were kept constant. The summary of the six-round design is given in Table 4 and Table 5. The simulation results are listed in Table 6 with estimated coefficients, t-ratios and p-values of each potential significant interaction. The analysis in Table 6 shows that the procedure identifies all insignificant interactions in the model. The t-values (p-values) provide the accepted adequacy of the estimated interactions in the simulation.

5 Conclusion

For a large system, resolution V design may be very difficult to construct. Our approach is to use a series of modified resolution IV designs and to estimate interactions involving one factor at a time. With no prior knowledge

Table 5: Random Level-setting of Constant Factors of the Six-round Design Strategy for Model(2)

Step	Row No.	Random Level-setting of constant factors
1	2	High: X_9 ; Low: X_{10}, X_{11}, X_{12}
2	4	High: $X_2, X_5, X_6, X_{11}, X_{12}$; Low: X_8, X_9, X_{10}
3	3	High: X_2, X_4 ; Low: X_{11}, X_{12}
4	1	High: X_3, X_{12} ; Low: X_2, X_4
5	6	High: $X_1, X_2, X_3, X_{10}, X_{11}$; Low: X_4, X_8, X_{12}
6	5	High: X_3, X_4 ; Low: X_1, X_2, X_6

of ISM, it needs a little more than n^2 runs to estimate all two factor interactions. The procedure has great advantages when prior knowledge of ISM is given. The procedure is very easy to program and use. It can deal with any system size. The difference from traditional fractional factorial design is that our procedure does not use all runs to estimate every interaction. Consequently, the estimates of interactions from our procedure have larger standard errors. However it is possible to iterate the procedure to reduce the standard error of the estimators of the interaction effects.

Table 6: Simulation Results for Model(2)

Interactions	Coefficients	t-values	p-values
X_1X_2	1.0049	74.02	0.000
X_1X_3	0.4902	30.19	0.000
X_1X_4	0.0166	0.650	0.536
X_1X_5	0.0260	1.310	0.207
X_1X_6	0.0070	0.360	0.721
X_1X_7	0.019	0.940	0.361
X_1X_8	-0.036	-1.800	0.091
X_1X_9	0.026	1.330	0.203
X_1X_{10}	-0.021	-1.060	0.304
X_1X_{11}	0.410	20.64	0.000
X_2X_3	0.0082	0.610	0.551
X_2X_4	0.2972	21.89	0.000
X_2X_5	-0.0011	-0.080	0.936
X_2X_6	0.2020	14.88	0.000
X_2X_7	-0.0236	-1.760	0.098
X_2X_8	-0.0134	-0.980	0.339
X_3X_4	0.1416	5.500	0.000
X_3X_5	-0.0275	-1.700	0.109
X_3X_6	0.0037	0.230	0.825
X_3X_7	-0.0061	-0.380	0.713
X_3X_8	-0.0133	-0.820	0.426
X_3X_9	-0.0090	-0.560	0.587
X_3X_{10}	0.0176	1.080	0.295
X_4X_7	0.0462	1.800	0.110
X_5X_6	-0.049	-1.93	0.090
X_5X_7	0.002	0.120	0.904
X_5X_8	0.015	0.870	0.397
X_5X_9	0.015	0.870	0.394
X_5X_{10}	0.031	1.810	0.087
X_5X_{11}	-0.001	-0.080	0.937
X_5X_{12}	0.003	0.180	0.857
X_6X_7	0.084	3.310	0.011
X_6X_9	-0.020	-0.780	0.456

Appendix

Proof of Theorem 1: For $n < 268 \pmod{4}$ Hadamard matrix has been constructed (See, for example, Paley(1933),Plackett and Burman (1964), Golomb and Hall (1962) and Raghavarao (1971)). Hence there exists an orthogonal resolution IV design for each n < 268.

Let n factors be X_1, X_2, \ldots, X_n and H be the resolution IV design matrix with dimension $2n \times n$ (Dey(1985)). Without lossing generalization assume i=1. Associate the columns of H to the main effects, say X_1 and all two-factor interactions involving X_1 , that is $X_1X_2, X_1X_3, \ldots, X_1X_n$, respectively. One may obtain the uniqe settings of X_1, X_2, \ldots, X_n by doing multplications of the first column by all other columns. Since H is resolution IV design estimates of X_1 and $X_1X_2, X_1X_3, \ldots, X_1X_n$ are free of other main effects and two-factor interactions. Now we show that this is minimal resolution IV designs. Since the design is to estimate $X_1, X_1X_2, X_1X_3, \ldots, X_1X_n$ free from other main and interaction effects $X_1, X_1X_2, X_1X_3, \ldots, X_1X_n$ is of full rank. Also grand mean, X_2, X_3, \ldots, X_n is of full rank by looking at the way of how to construct X_2, X_3, \ldots, X_n from $X_1, X_1X_2, X_1X_3, \ldots, X_1X_n$. Recall this design is to estimate $X_1, X_1X_2, X_1X_3, \ldots, X_1X_n$ and grand mean, X_2, X_3, \ldots, X_n we have 2n vectors $X_1, X_1X_2, X_1X_3, \ldots, X_1X_n$ and grand mean, X_2, X_3, \ldots, X_n are independent. So we at least need 2n experimental runs.

Proof of Theorem 2: Conduct the modified resolution IV design discussed in above theorem n times. Each time one obtains the completely estimations for one factor (including the main effect and all two-factor interactions involving this factor). After each step the number of factors decreases by 1 by letting this factor be constant. Let n = 4m + k, where m is an integer and k = 0, 1, 2, 3. For $m \ge 1$, the total number of experimental runs needed is equal to $8k(m+1) + 32(m+...+2) + 8 + 8 + 4 = 8k(m+1) + 16m(m+1) - 12 = n^2 + 4n - k^2 + 4k - 12 \le n^2 + 4n - 8$.

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